

FILE 'REGISTRY' ENTERED AT 11:09:29 ON 03 JUN 2002
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STRUCTURE FILE UPDATES: 2 JUN 2002 HIGHEST RN 424787-52-0
DICTIONARY FILE UPDATES: 2 JUN 2002 HIGHEST RN 424787-52-0

TSCA INFORMATION NOW CURRENT THROUGH January 7, 2002

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES
for more information. See STNote 27, Searching Properties in the CAS
Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

Uploading rkc660.str

L1 STRUCTURE UPLOADED

=> s l1

SAMPLE SEARCH INITIATED 11:13:49 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 0 TO 0
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 ful

FULL SEARCH INITIATED 11:13:55 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1

=>

Uploading rkc660.str

L4 STRUCTURE UPLOADED

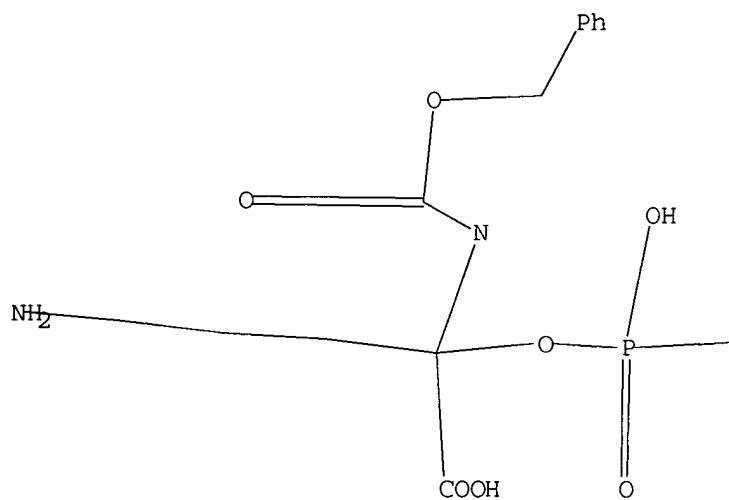
=> s l4 ful

FULL SEARCH INITIATED 11:15:30 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L5 0 SEA SSS FUL L4

=> d
L5 HAS NO ANSWERS
L4 STR



Structure attributes must be viewed using STN Express query preparation.
L5 0 SEA FILE=REGISTRY SSS FUL L4

=>

=>

Executing the logoff script...

=> LOG H

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION






FULL ESTIMATED COST

283.60

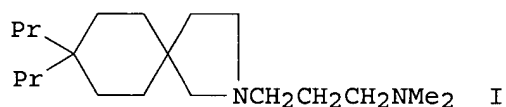
283.81

SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 11:15:44 ON 03 JUN 2002

-  L1: (0) benzyloxycarbonylamino and phosphinoxy and pentanoic
-  L2: (3) phosphinoyl and pentanoic
-  L4: (0) 13 and phosphinoyl
-  L3: (192) benzyloxycarbonylamino and pentanoic
-  L5: (23) 13 and phosphine

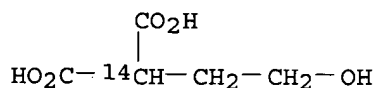
AN 1995:911404 CAPLUS
 DN 124:145795
 TI Synthesis of .gamma.-butyrolactone-[2-14C] and its use in the synthesis of an immunomodulatory azaspirane
 AU Landvatter, Scott W.; Garnes, Keith T.; Heys, J. Richard; Beecham, SmithKline
 CS Radiochemistry Section, Synthetic Chemistry Department, King of Prussia, PA, 19406, USA
 SO Synthesis and Applications of Isotopically Labelled Compounds 1994, Proceedings of the International Symposium, 5th, Strasbourg, June 20-24, 1994 (1995), Meeting Date 1994, 631-4. Editor(s): Allen, John; Voges, Rolf. Publisher: Wiley, Chichester, UK.
 CODEN: 61UMAF
 DT Conference
 LA English
 GI



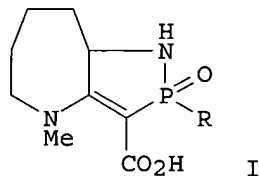
AB SK&F 105685 (I) is a novel immunomodulatory azaspirane that was investigated for the treatment of rheumatoid arthritis. Synthesis of the mol. with carbon-14 in one of the ring carbons not adjacent to nitrogen was required for metab. studies. The key intermediate in the synthesis of I was the prepn. of .gamma.-butyrolactone (7) labeled in the 2 position. Alkylation of di-Et malonate-[2-14C] with 1-bromo-2-(phenylmethoxy)ethane followed by sapon. gave the monoalkylated malonic acid deriv. Debenzylation by catalytic hydrogenation and subsequent decarboxylation gave the desired .gamma.-butyrolactone-[2-14C] (7) in 58% overall radiochem. yield from di-Et malonate-[2-14C]. Conversion to the lactam was readily achieved by heating at 230.degree.C with the neat amine. Final conversion to the target mol. gave I with the carbon-14 at the spiro carbon. Several other possible routes to the lactone 7 were also investigated. None of these alternatives (alkylation of di-Et malonate with ethylene oxide, chloroethanol, or ethylene carbonate; partial redn. of succinic anhydride) gave satisfactory results, however.

IT 173163-00-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (synthesis of .gamma.-butyrolactone-[2-14C] and its use in the synthesis of an immunomodulatory azaspirane)

RN 173163-00-3 CAPLUS
 CN Propanedioic-2-14C acid, 2-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)



L9 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS
 AN 1992:490722 CAPLUS
 DN 117:90722
 TI Condensation of phosphono-, phosphinoacetic acid and lactam acetal of
 L-lysine and enzyme catalyzed cyclization
 AU Nachev, I. A.
 CS Res. Cent. "Konstrukcionni Polymeri", Sofia, 1528, Bulg.
 SO Izvestiya po Khimiya (1991), 24(1), 18-25
 CODEN: IZKHDX; ISSN: 0324-0401
 DT Journal
 LA English
 GI



AB The condensation of $\text{RP(O)(OEt)CH}_2\text{CO}_2\text{Et}$ type of esters ($\text{R} = \text{OEt}$ or Me) and $\text{R}_1\text{C(OR}_2\text{)}_2\text{NR}_3$ type of acetals in the presence of $\text{BF}_3 \cdot \text{Et}_2\text{O}$ was carried out to give $\text{RP(O)(OEt)CH(R}_2\text{)CO}_2\text{Et}$, $\text{RP(O)(OEt)C(CO}_2\text{Et):CR}_1\text{NR}_3$, and R_2OH ($\text{R}_1 = \text{e.g., Me, R}_2 = \text{Et}$) resp. It was established that the enzyme phosphodiesterase I contributes to the formation of the azaphospholane rings in I ($\text{R} = \text{OH}$ or Me).

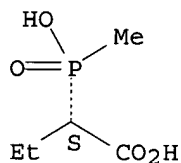
IT 142795-22-0P

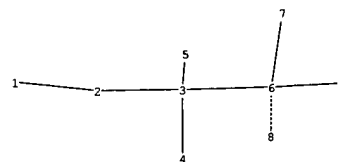
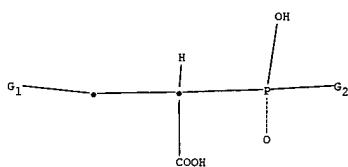
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 142795-22-0 CAPLUS

CN Butanoic acid, 2-(hydroxymethylphosphinyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.





chain nodes :

1 2 3 4 5 6 7 8 9

chain bonds :

1-2 2-3 3-4 3-5 3-6 6-7 6-8 6-9

exact/norm bonds :

1-2 6-7 6-8 6-9

exact bonds :

2-3 3-4 3-5 3-6

G1:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

G2:N,CH3,Et,n-Pr,i-Pr,n-Bu,t-Bu

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS